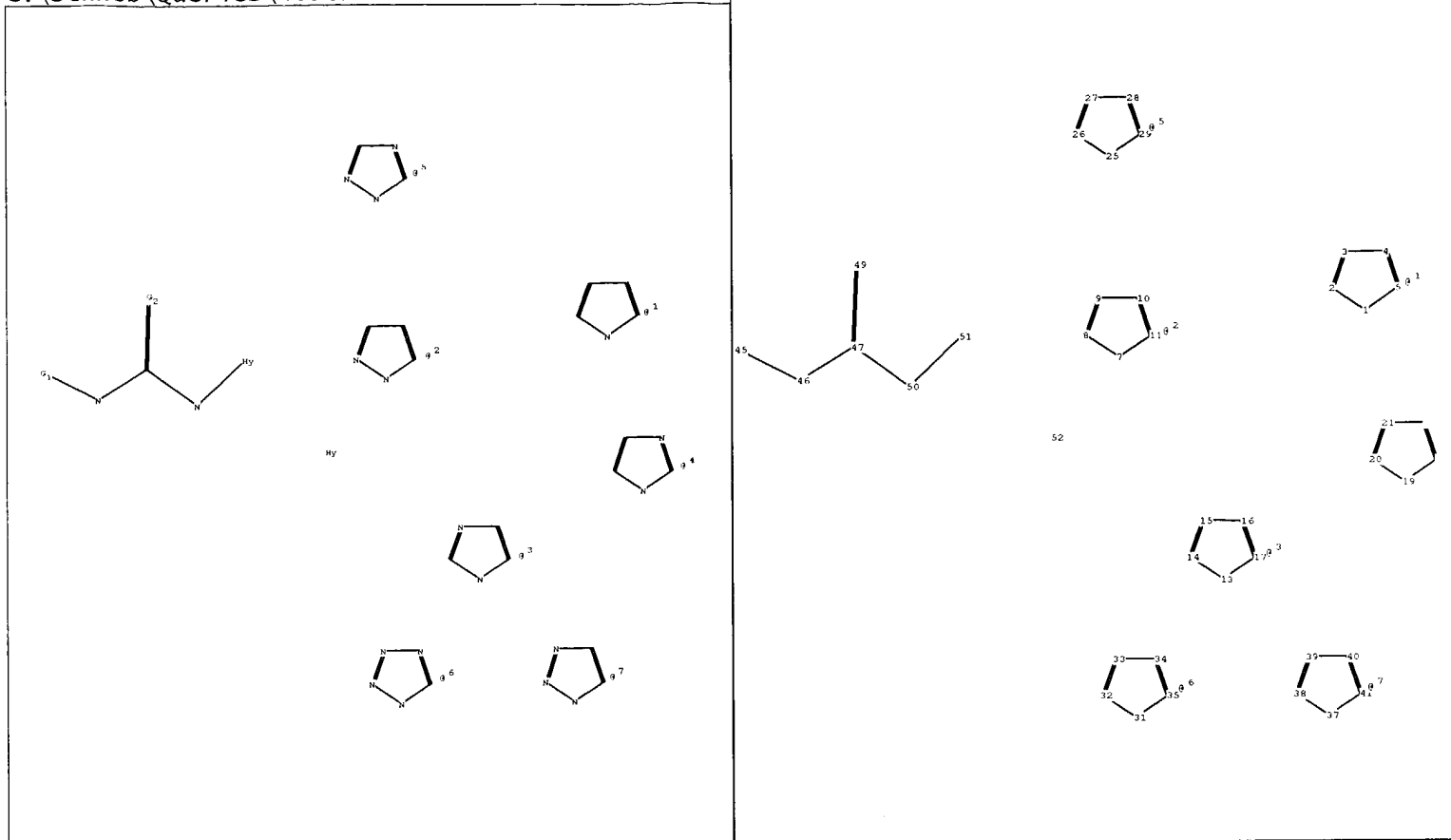C:\stnweb\Queries\4.str

chain nodes :
    45   46   47   49   50   51   52
ring nodes :
    1   2   3   4   5   7   8   9   10   11   13   14   15   16   17   19   20   21   22   23   25   26   27   28
    29   31   32   33   34   35   37   38   39   40   41
chain bonds :
    45-46   46-47   47-49   47-50   50-51
ring bonds :
    1-2   1-5   2-3   3-4   4-5   7-8   7-11   8-9   9-10   10-11   13-14   13-17   14-15   15-16   16-17
    19-20   19-23   20-21   21-22   22-23   25-26   25-29   26-27   27-28   28-29   31-32   31-35   32-33
    33-34   34-35   37-38   37-41   38-39   39-40   40-41
exact/norm bonds :
    1-2   1-5   7-8   7-11   8-9   13-14   13-17   14-15   15-16   19-20   19-23   20-21   21-22   22-23
    25-26   25-29   26-27   27-28   28-29   31-32   31-35   32-33   33-34   34-35   37-38   37-41   38-39
    39-40   45-46   46-47   47-49   47-50   50-51
exact bonds :
    2-3   3-4   4-5   9-10   10-11   16-17   40-41
isolated ring systems :
    containing 1 : 7 : 13 : 25 : 31 : 37 :

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

G2:O,S

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:CLASS   11:Atom
    13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom   23:Atom
    25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   31:Atom   32:Atom   33:Atom   34:Atom   35:Atom
    37:Atom   38:Atom   39:Atom   40:Atom   41:Atom   45:CLASS   46:CLASS   47:CLASS   49:CLASS
    50:CLASS   51:Atom   52:Atom
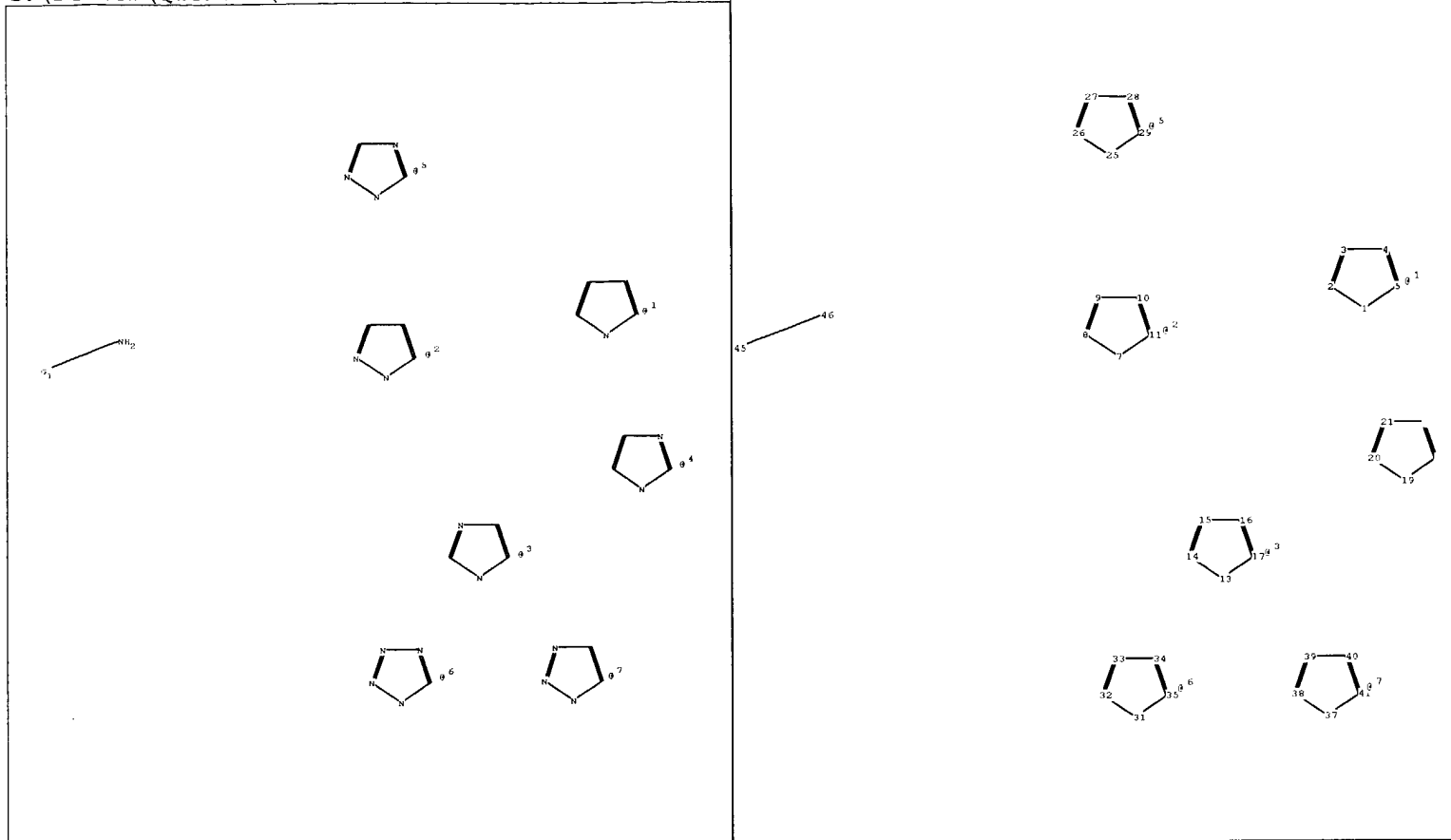
```
chain nodes :
    45  46
ring nodes :
    1   2   3   4   5   7   8   9   10  11  13  14  15  16  17  19  20  21  22  23  25  26  27  28
    29  31  32  33  34  35  37  38  39  40  41
chain bonds :
    45-46
ring bonds :
    1-2   1-5   2-3   3-4   4-5   7-8   7-11  8-9   9-10  10-11  13-14  13-17  14-15  15-16  16-17
    19-20  19-23  20-21  21-22  22-23  25-26  25-29  26-27  27-28  28-29  31-32  31-35  32-33
    33-34  34-35  37-38  37-41  38-39  39-40  40-41
exact/norm bonds :
    1-2   1-5   7-8   7-11  8-9   13-14  13-17  14-15  15-16  19-20  19-23  20-21  21-22  22-23
    25-26  25-29  26-27  27-28  28-29  31-32  31-35  32-33  33-34  34-35  37-38  37-41  38-39
    39-40  45-46
exact bonds :
    2-3   3-4   4-5   9-10  10-11  16-17  40-41
isolated ring systems :
    containing 1 : 7 : 13 : 25 : 31 : 37 :


G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   7:Atom   8:Atom   9:Atom   10:CLASS   11:Atom
    13:Atom   14:Atom   15:Atom   16:Atom   17:Atom   19:Atom   20:Atom   21:Atom   22:Atom   23:Atom
    25:Atom   26:Atom   27:Atom   28:Atom   29:Atom   31:Atom   32:Atom   33:Atom   34:Atom   35:Atom
    37:Atom   38:Atom   39:Atom   40:Atom   41:Atom   45:CLASS   46:CLASS
```
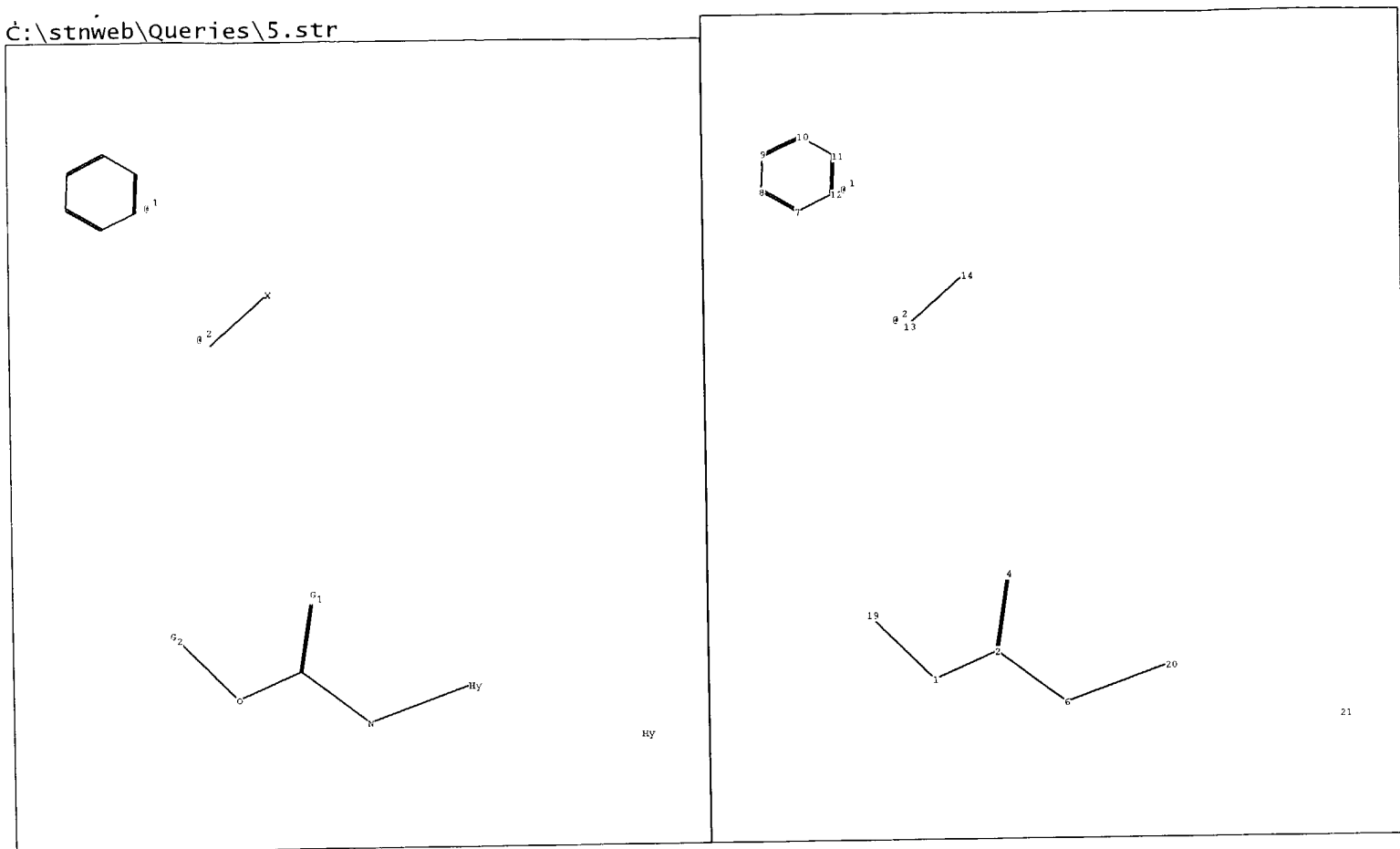
chain nodes :
    1   2   4   6   13   14   19   20   21
ring nodes :
    7   8   9   10   11   12
chain bonds :
    1-2   1-19   2-4   2-6   6-20   13-14
ring bonds :
    7-8   7-12   8-9   9-10   10-11   11-12
exact/norm bonds :
    1-2   1-19   2-4   2-6   6-20
exact bonds :
    13-14
normalized bonds :
    7-8   7-12   8-9   9-10   10-11   11-12
isolated ring systems :
    containing 7 :

G1:O,S

G2:[*1],[*2]

Match level :
    1:CLASS   2:CLASS   4:CLASS   6:CLASS   7:Atom   8:Atom   9:Atom   10:Atom   11:Atom   12:Atom
    13:CLASS   14:CLASS   19:CLASS   20:Atom   21:Atom

```
* * * * * * * * *    Welcome to STN International    * * * * * * * * * *
```

NEWS   1   Web Page URLs for STN Seminar Schedule - N. America
NEWS   2   "Ask CAS" for self-help around the clock
NEWS   3   May 10   PROUSDDR now available on STN
NEWS   4   May 19   PROUSDDR: One FREE connect hour, per account, in both May
                      and June 2004
NEWS   5   May 12   EXTEND option available in structure searching
NEWS   6   May 12   Polymer links for the POLYLINK command completed in REGISTRY
NEWS   7   May 17   FRFULL now available on STN
NEWS   8   May 27   STN User Update to be held June 7 and June 8 at the SLA 2004
                      Conference
NEWS   9   May 27   New UPM (Update Code Maximum) field for more efficient patent
                      SDIs in CAplus
NEWS 10   May 27   CAplus super roles and document types searchable in REGISTRY
NEWS 11   May 27   Explore APOLLIT with free connect time in June 2004

NEWS EXPRESS   MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
                MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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     * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

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DICTIONARY FILE UPDATES: 17 JUN 2004   HIGHEST RN 694921-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e isoquinoline/cn
E1          1       ISOQUINOLIN-7-YL TRIFLUOROMETHANESULFONATE/CN
E2          1       ISOQUINOLINAMINE, 1,3-DICHLORO-/CN
E3          1 -->   ISOQUINOLINE/CN
E4          1       ISOQUINOLINE 1-(3-(BENZYLOXY)-4-METHOXYBENZYL)-3,4-DIHYDRO-6
                     -METHOXY-, PICRATE/CN
E5          1       ISOQUINOLINE 1-OXIDOREDUCTASE/CN
E6          1       ISOQUINOLINE 1-OXIDOREDUCTASE (ALPHA SUBUNIT) OXIDOREDUCTASE
                     PROTEIN (RALSTONIA SOLANACEARUM STRAIN GMI1000 GENE IORA2)/
                     CN
E7          1       ISOQUINOLINE 1-OXIDOREDUCTASE (CHROMOBACTERIUM VIOLACEUM STR
                    AIN ATCC 12472 GENE CV1674)/CN
E8          1       ISOQUINOLINE 1-OXIDOREDUCTASE (PSEUDOMONAS PUTIDA STRAIN KT2
                    440 GENE PP3947)/CN
E9          1       ISOQUINOLINE 1-OXIDOREDUCTASE (SHEWANELLA ONEIDENSIS STRAIN
                    MR-1 GENE SO3048 BETA SUBUNIT)/CN
E10         1       ISOQUINOLINE 1-OXIDOREDUCTASE (SHEWANELLA ONEIDENSIS STRAIN
                    MR-1 GENE SO3049 ALPHA SUBUNIT)/CN
E11         1       ISOQUINOLINE 1-OXIDOREDUCTASE, ALPHA SUBUNIT (CAULOBACTER CR
                    ESCENTUS GENE CC0022)/CN
E12         1       ISOQUINOLINE 1-OXIDOREDUCTASE, ALPHA SUBUNIT (CAULOBACTER CR
                    ESCENTUS GENE CC2270)/CN

=> s e3
L1          1 ISOQUINOLINE/CN

=> d l1

L1    ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN    119-65-3  REGISTRY
CN    Isoquinoline (6CI, 8CI, 9CI)   (CA INDEX NAME)
OTHER NAMES:
CN    β-Quinoline
CN    2-Azanaphthalene
CN    2-Benzazine
CN    Benzopyridine
CN    Benzo[c]pyridine
CN    NSC 3395
FS    3D CONCORD
MF    C9 H7 N
CI    COM, RPS
LC    STN Files:   ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS,
         BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN,
         CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*,
         DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2,
         GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*,
         MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO,
         TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL
            (*File contains numerically searchable property data)
         Other Sources:  DSL**, EINECS**, TSCA**
            (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA  CAplus document type:  Book; Conference; Dissertation; Journal; Patent;
         Preprint; Report
```

RL.P   Roles from patents: ANST (Analytical study); BIOL (Biological study);
        MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP
        (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in
        record)
RLD.P   Roles for non-specific derivatives from patents: ANST (Analytical
        study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation);
        PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
        (Uses)
RL.NP   Roles from non-patents: ANST (Analytical study); BIOL (Biological
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        (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
        (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical
        study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC
        (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);
        PRP (Properties); RACT (Reactant or reagent); USES (Uses)
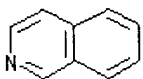
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

        4006 REFERENCES IN FILE CA (1907 TO DATE)
         366 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
        4012 REFERENCES IN FILE CAPLUS (1907 TO DATE)
           9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=>
L2   STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2   STR

=> s l2
SAMPLE SEARCH INITIATED 16:34:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   661 TO ITERATE

100.0% PROCESSED   661 ITERATIONS   2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 11678 TO   14762
PROJECTED ANSWERS: 2 TO   124

L3   2 SEA SSS SAM L2

=> s l2 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:34:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13265 TO ITERATE

100.0% PROCESSED   13265 ITERATIONS   43 ANSWERS
SEARCH TIME: 00.00.01

L4   43 SEA SSS FUL L2

=> file hcaplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                           ENTRY   SESSION
FULL ESTIMATED COST   170.44   170.65

FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
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FILE COVERS 1907 - 18 Jun 2004   VOL 140 ISS 26
FILE LAST UPDATED: 17 Jun 2004   (20040617/ED)

 This file contains CAS Registry Numbers for easy and accurate
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=> s 14/prep
          15 L4
     3160985 PREP/RL
L5   13 L4/PREP
             (L4 (L) PREP/RL)

=> s 15 and tan, Z?/au
        1084 TAN, Z?/AU
L6   0 L5 AND TAN, Z?/AU

=> s 15 and song, j?/au
        4830 SONG, J?/AU
L7   0 L5 AND SONG, J?/AU

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                           ENTRY   SESSION
FULL ESTIMATED COST   7.08   177.73

FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
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STRUCTURE FILE UPDATES: 17 JUN 2004   HIGHEST RN 694921-36-3
DICTIONARY FILE UPDATES: 17 JUN 2004   HIGHEST RN 694921-36-3

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http://www.cas.org/ONLINE/DBSS/registryss.html

```
=>
L8        STRUCTURE UPLOADED

=> d 18
L8 HAS NO ANSWERS
L8                STR

=> s 18
SAMPLE SEARCH INITIATED 16:38:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  24419 TO ITERATE

  4.1% PROCESSED    1000 ITERATIONS                          49 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **INCOMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:      479039 TO    497721
PROJECTED ANSWERS:          21855 TO     26005

L9            49 SEA SSS SAM L8

=>
L10       STRUCTURE UPLOADED

=> d 110
L10 HAS NO ANSWERS
L10                STR
  0 16 S 17
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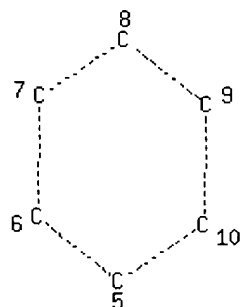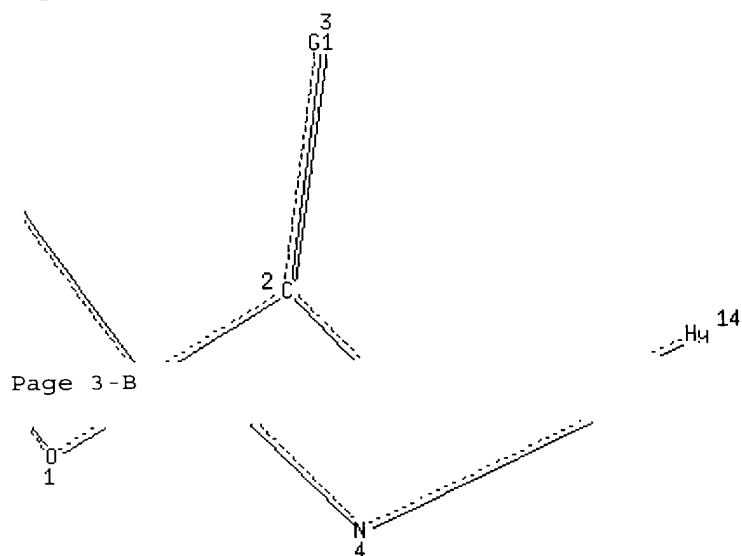

Page 1-A

Page 1-B

11 C

Page 2-B

13 G2

Page 3-A

3
G1

2 C

Hʉ 14

Page 3-B

O
1

N
4

Page 4-B

Hʉ 15

Page 4-C

VAR G1=16/17
VAR G2=10/11
NODE ATTRIBUTES:
NSPEC   IS C   AT   1
NSPEC   IS C   AT   2
NSPEC   IS C   AT   3
NSPEC   IS C   AT   4
NSPEC   IS R   AT   5
NSPEC   IS R   AT   6
NSPEC   IS R   AT   7
NSPEC   IS R   AT   8
NSPEC   IS R   AT   9
NSPEC   IS R   AT 10
NSPEC   IS C   AT 11
NSPEC   IS C   AT 12
NSPEC   IS C   AT 13
NSPEC   IS C   AT 14
NSPEC   IS C   AT 15
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS AT   1   2   4 11 12 16 17
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I

NUMBER OF NODES IS   17

STEREO ATTRIBUTES: NONE

=> s l10
SAMPLE SEARCH INITIATED 16:41:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3872 TO ITERATE

 25.8% PROCESSED   1000 ITERATIONS   8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 73709 TO   81171
PROJECTED ANSWERS: 286 TO   952

L11   8 SEA SSS SAM L10

=> s l10 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:41:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   77434 TO ITERATE

100.0% PROCESSED   77434 ITERATIONS   387 ANSWERS
SEARCH TIME: 00.00.02

L12   387 SEA SSS FUL L10

=> file hcaplus   SINCE FILE   TOTAL
COST IN U.S. DOLLARS   ENTRY   SESSION
                                                 158.36   336.09
FULL ESTIMATED COST

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FILE LAST UPDATED: 17 Jun 2004 (20040617/ED)

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 substance identification.

=> s l12/rct

```
            222 L12
        2631689 RCT/RL
L13          69 L12/RCT
                (L12 (L) RCT/RL)


=> d his

        (FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004)

        FILE 'REGISTRY' ENTERED AT 16:21:32 ON 18 JUN 2004
                    E ISOQUINOLINE/CN
L1           1 S E3
L2             STRUCTURE UPLOADED
L3           2 S L2
L4          43 S L2 FULL


        FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
L5          13 S L4/PREP
L6           0 S L5 AND TAN, Z?/AU
L7           0 S L5 AND SONG, J?/AU


        FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
L8             STRUCTURE UPLOADED
L9          49 S L8
L10            STRUCTURE UPLOADED
L11          8 S L10
L12        387 S L10 FULL


        FILE 'HCAPLUS' ENTERED AT 16:41:29 ON 18 JUN 2004
L13         69 S L12/RCT


=> s l13 and l5
L14          0 L13 AND L5


=> file caold
COST IN U.S. DOLLARS                     SINCE FILE      TOTAL
                                           ENTRY       SESSION
FULL ESTIMATED COST                        2.36         338.45
```

FILE 'CAOLD' ENTERED AT 16:41:59 ON 18 JUN 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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   now searchable from 1907-1966. TIFF images of CA abstracts
   printed between 1907-1966 are available in the PAGE
   display formats.

   This file supports REG1stRY for direct browsing and searching of
   all substance data from the REGISTRY file. Enter HELP FIRST for
   more information.

=> d his

```
            (FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004)

            FILE 'REGISTRY' ENTERED AT 16:21:32 ON 18 JUN 2004
                        E ISOQUINOLINE/CN
L1              1 S E3
L2                STRUCTURE UPLOADED
L3              2 S L2
L4             43 S L2 FULL


            FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
L5             13 S L4/PREP
L6              0 S L5 AND TAN, Z?/AU
L7              0 S L5 AND SONG, J?/AU


            FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
L8                STRUCTURE UPLOADED
L9             49 S L8
L10               STRUCTURE UPLOADED
L11             8 S L10
L12           387 S L10 FULL


            FILE 'HCAPLUS' ENTERED AT 16:41:29 ON 18 JUN 2004
L13            69 S L12/RCT
L14             0 S L13 AND L5

            FILE 'CAOLD' ENTERED AT 16:41:59 ON 18 JUN 2004

=> s 14 and 112
                0 L4
                6 L12
L15             0 L4 AND L12

=>
```